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Bis(1-methyl-1-phenylethyl) peroxide

Wei-Yi Su, Guang-Yang Hou, Qiu-Xiang Yin* and Li-Na Zhou

School of Chemical Engineering and Technology, Tianjin University, Tianjin 300072, People's Republic of China
Correspondence e-mail: suweiyi222@yahoo.com.cn

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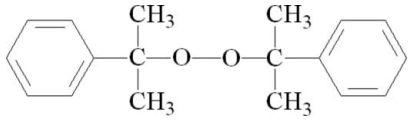
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.110; data-to-parameter ratio = 15.9.

In the crystal structure, the title compound (also called dicumyl peroxide), $C_{18}H_{22}O_2$, lies on a center of symmetry. The COOC plane including the dioxy group makes a dihedral angle of 79.10 (5)° with the phenyl ring. An intermolecular C—H$\cdots\pi$ interaction is observed between the phenyl groups.

Related literature

For general background, see: Ferrero (2006); Konar *et al.* (1993); Ramar & Alagar (2004); Wang *et al.* (1998).



Experimental

Crystal data

$C_{18}H_{22}O_2$
M_r = 270.36
Orthorhombic, *Pbca*
a = 10.040 (2) Å
b = 7.4774 (15) Å
c = 21.016 (4) Å
V = 1577.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
0.25 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.982, T_{max} = 0.989
11957 measured reflections
1464 independent reflections
1232 reflections with $I > 2\sigma(I)$
R_{int} = 0.077

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.110
S = 1.05
1464 reflections
92 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

Cg is the centroid of the phenyl ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C3—H3$A\cdots Cg^{i}$	0.93	2.93	3.7874 (17)	154

Symmetry code: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *RAPID-AUTO* (Rigaku/MSC, 2004); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2340).

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supporting information

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Bis(1-methyl-1-phenylethyl) peroxide

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S1. Comment

The title compound, (I), a simple organic peroxide, has gradually become almost the most important additive in operations affected by molecular transport, such as grafting (Konar *et al.*, 1993; Ramar & Alagar, 2004) and cross-linking (Wang *et al.*, 1998; Ferrero, 2006), which are based on the formation of oxyradicals due to the thermal decomposition of the peroxides. It's widely used in the art as vulcanizing agents for resins and elastomers, as cross-linking agents for polyolefins.

The centrosymmetric molecular structure of (I) is shown in Fig. 1. In the molecule, two phenyl rings are, of course, parallel to each other due to the symmetry element. The peroxy unit has an O—O bond length of 1.6853 (16) Å, and the four atoms, C7, O1, O1A and C7A are coplanar with a C7—O1—O1A bond angle of 106.02 (9)°. There is no hydrogen bond in the packing structure, and cohesion of the crystal can be attributed to van der Waals interactions.

S2. Experimental

At room temperature, the title compound (1 g) provided by Gaoqiao petrochemical corporation was dissolved in 20 mL ethanol (99.7%). The solvent was vaporized slowly by use of a film covering the container (beaker). Then the solution was placed in darkness until crystals appeared. The product was taken out from the solvent by tweezers, and dried in the air at room temperature.

S3. Refinement

H atoms are placed in calculated positions and constrained to ride on their parent atoms, with C–H = 0.93–0.96 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

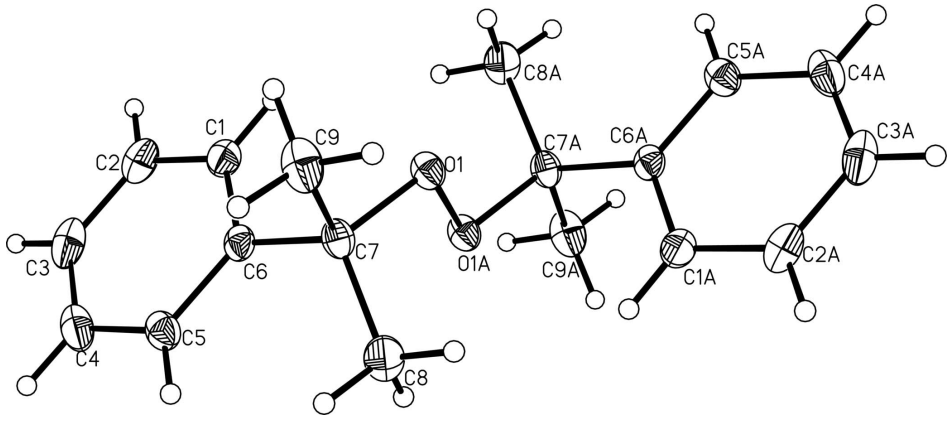

Figure 1

The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

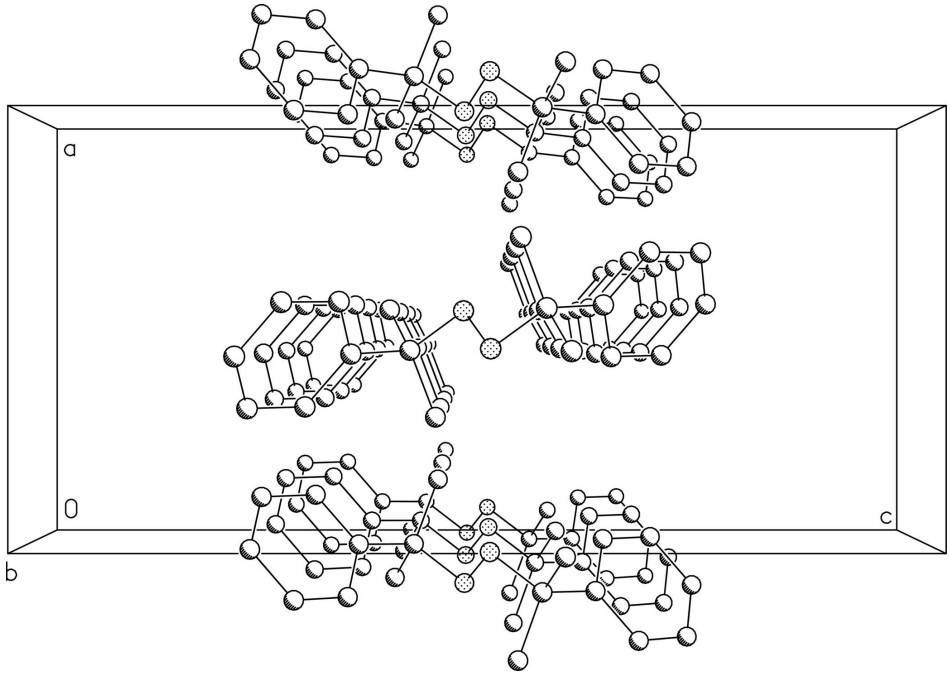

Figure 2

The packing diagram of (I), viewed down the *b* axis. H atoms have been omitted.

Bis(1-methyl-1-phenylethyl) peroxide

Crystal data

$C_{18}H_{22}O_2$
$M_r = 270.36$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 10.040\ (2)$ Å
$b = 7.4774\ (15)$ Å
$c = 21.016\ (4)$ Å
$V = 1577.7\ (5)$ Å^3
$Z = 4$
$F(000) = 584$
$D_x = 1.138$ Mg m^{-3}
Melting point: 315.15 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 8972 reflections
$\theta = 3.5$–$27.6°$
$\mu = 0.07$ mm^{-1}
$T = 293$ K
Plate, colorless
0.25 × 0.20 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID IP area-detector diffractometer
Radiation source: rotating anode
Graphite monochromator
oscillation scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.982$, $T_{max} = 0.989$
11957 measured reflections
1464 independent reflections
1232 reflections with $I > 2\sigma(I)$
$R_{int} = 0.077$
$\theta_{max} = 25.5°$, $\theta_{min} = 3.5°$
$h = -12 \rightarrow 10$
$k = -9 \rightarrow 9$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.110$
$S = 1.05$
1464 reflections
92 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 0.2734P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.010$
$\Delta\rho_{max} = 0.26$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.027 (7)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.46269 (8)	0.07789 (11)	0.51277 (4)	0.0309 (3)
C1	0.44577 (13)	−0.10967 (18)	0.62787 (6)	0.0373 (4)
H1A	0.3746	−0.1115	0.5996	0.045*
C2	0.44768 (16)	−0.2285 (2)	0.67854 (6)	0.0462 (4)
H2A	0.3785	−0.3099	0.6836	0.055*
C3	0.55144 (16)	−0.2265 (2)	0.72135 (6)	0.0482 (4)
H3A	0.5527	−0.3060	0.7554	0.058*
C4	0.65322 (16)	−0.1055 (2)	0.71319 (6)	0.0453 (4)
H4A	0.7231	−0.1025	0.7422	0.054*
C5	0.65252 (13)	0.01215 (17)	0.66204 (6)	0.0353 (3)
H5A	0.7227	0.0920	0.6568	0.042*
C6	0.54838 (12)	0.01186 (16)	0.61873 (5)	0.0285 (3)
C7	0.54171 (12)	0.14706 (16)	0.56434 (6)	0.0302 (3)
C8	0.67730 (14)	0.20577 (19)	0.54013 (6)	0.0419 (4)
H8A	0.7274	0.1027	0.5271	0.063*
H8B	0.7242	0.2670	0.5734	0.063*
H8C	0.6660	0.2847	0.5045	0.063*
C9	0.45933 (16)	0.30860 (19)	0.58538 (6)	0.0457 (4)
H9A	0.3740	0.2689	0.6004	0.068*
H9B	0.4472	0.3880	0.5500	0.068*
H9C	0.5051	0.3703	0.6190	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0353 (5)	0.0293 (5)	0.0282 (5)	0.0064 (4)	−0.0042 (4)	−0.0065 (3)
C1	0.0372 (7)	0.0434 (8)	0.0312 (7)	−0.0045 (6)	0.0036 (6)	0.0002 (6)
C2	0.0558 (9)	0.0452 (9)	0.0377 (8)	−0.0046 (7)	0.0142 (7)	0.0028 (6)
C3	0.0711 (11)	0.0426 (9)	0.0309 (7)	0.0163 (7)	0.0120 (7)	0.0058 (6)
C4	0.0556 (9)	0.0506 (9)	0.0297 (7)	0.0182 (7)	−0.0080 (7)	−0.0051 (6)
C5	0.0383 (7)	0.0358 (7)	0.0319 (7)	0.0045 (6)	−0.0042 (6)	−0.0074 (5)
C6	0.0330 (7)	0.0288 (7)	0.0235 (6)	0.0042 (5)	0.0017 (5)	−0.0057 (5)
C7	0.0377 (7)	0.0271 (6)	0.0258 (6)	−0.0014 (5)	−0.0039 (5)	−0.0034 (5)
C8	0.0495 (8)	0.0387 (8)	0.0376 (7)	−0.0153 (6)	−0.0015 (7)	0.0017 (6)
C9	0.0654 (10)	0.0339 (8)	0.0377 (8)	0.0124 (7)	−0.0072 (7)	−0.0068 (6)

Geometric parameters (Å, º)

O1—C7	1.4392 (15)	C5—C6	1.3862 (17)
O1—O1^{i}	1.4853 (16)	C5—H5A	0.9300
C1—C6	1.3871 (18)	C6—C7	1.5273 (17)
C1—C2	1.387 (2)	C7—C8	1.5181 (18)
C1—H1A	0.9300	C7—C9	1.5292 (18)
C2—C3	1.377 (2)	C8—H8A	0.9600
C2—H2A	0.9300	C8—H8B	0.9600
C3—C4	1.375 (2)	C8—H8C	0.9600
C3—H3A	0.9300	C9—H9A	0.9600
C4—C5	1.3893 (19)	C9—H9B	0.9600
C4—H4A	0.9300	C9—H9C	0.9600
C7—O1—O1^{i}	106.02 (9)	O1—C7—C8	110.23 (10)
C6—C1—C2	121.05 (13)	O1—C7—C6	110.47 (10)
C6—C1—H1A	119.5	C8—C7—C6	113.76 (10)
C2—C1—H1A	119.5	O1—C7—C9	101.74 (10)
C3—C2—C1	120.35 (14)	C8—C7—C9	110.70 (11)
C3—C2—H2A	119.8	C6—C7—C9	109.28 (10)
C1—C2—H2A	119.8	C7—C8—H8A	109.5
C4—C3—C2	119.21 (14)	C7—C8—H8B	109.5
C4—C3—H3A	120.4	H8A—C8—H8B	109.5
C2—C3—H3A	120.4	C7—C8—H8C	109.5
C3—C4—C5	120.61 (13)	H8A—C8—H8C	109.5
C3—C4—H4A	119.7	H8B—C8—H8C	109.5
C5—C4—H4A	119.7	C7—C9—H9A	109.5
C6—C5—C4	120.72 (13)	C7—C9—H9B	109.5
C6—C5—H5A	119.6	H9A—C9—H9B	109.5
C4—C5—H5A	119.6	C7—C9—H9C	109.5
C5—C6—C1	118.05 (12)	H9A—C9—H9C	109.5
C5—C6—C7	121.56 (11)	H9B—C9—H9C	109.5
C1—C6—C7	120.31 (11)		

C6—C1—C2—C3	0.7 (2)	O1^{i}—O1—C7—C6	−65.93 (12)
C1—C2—C3—C4	−0.1 (2)	O1^{i}—O1—C7—C9	178.12 (10)
C2—C3—C4—C5	−0.7 (2)	C5—C6—C7—O1	155.72 (11)
C3—C4—C5—C6	0.95 (19)	C1—C6—C7—O1	−27.54 (15)
C4—C5—C6—C1	−0.32 (18)	C5—C6—C7—C8	31.13 (16)
C4—C5—C6—C7	176.48 (11)	C1—C6—C7—C8	−152.13 (12)
C2—C1—C6—C5	−0.51 (19)	C5—C6—C7—C9	−93.14 (14)
C2—C1—C6—C7	−177.36 (12)	C1—C6—C7—C9	83.59 (14)
O1^{i}—O1—C7—C8	60.64 (13)		

Symmetry code: (i) −*x*+1, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3*A*···*Cg*^{ii}	0.93	2.93	3.7874 (17)	154

Symmetry code: (ii) −*x*+1, *y*−1/2, −*z*+3/2.